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ITOUGH2 V3.2

Verification and Validation Report

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DISCLAIMER

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1 . Introduction

This report describes the Verification and Validation (V & V) test cases performed to qualify ITOUGH2 V3.2 in compliance with YMP-LBNL-QIP-SI.0, Rev. 3, Mod. 0. The testing of the software follows the V & V Plan as outlined in SCMS Form 3, Point 1, and addresses the functional requirements given in SCMS Form 2, Point 4.

The qualification of software related to ITOUGH2 is described in *Pruess et al.* [1996], *Wu et al.* [1996], and *Finsterle et al.* [1996].

The requirements are reproduced in Table 1.1. Additional information can be found in the user's manual [*Finsterle*, 1998].

Table 1.1. List of Requirements

#	Requirement	Section
	Fracture-matrix interface area reduced by:	
1.1	A constant	2.1.1
1.2	Upstream saturation	2.1.2
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ITOUGH2 V3.2 was installed in a directory ~/itough2v3.2 on a SUN ULTRA 1 workstation under UNIX Solaris 2. Instructions for installing ITOUGH2 can be found in file *read.me* and the user's manual.

This report is structured as follows: For each functional requirement, the corresponding design is described, which may include the mathematical model implemented in ITOUGH2 V3.2, if appropriate. Next, we discuss the test case or sequence of test cases performed to validate each requirement, followed by a description of the test results and their compliance with the acceptance criteria given in SCMS Form 3, Point 1.

2. Test Results

2.1 Fracture-Matrix Interface Area Reduction

There is evidence that fracture-matrix interaction in the unsaturated zone is reduced as a result of fracture coatings as well as preferential flow in the fractures as induced by flow instabilities (fingering) and small-scale heterogeneities. A number of options for reducing fracture-matrix interface area have been implemented for use in a dual-permeability flow simulation. Interface area reduction is applied to connections with a negative value for variable `ISOT`, which is provided in the CONNE block [*Pruess*, 1987]. Different modifiers are used depending on the value of `ISOT` and `MOP(8)` as summarized in Table 2.1.1.

Table 2.1.1. Option for Reducing Fracture-Matrix Interface Area

`ISOT`	`MOP(8)`	Interface area reduction factor a_{fm}
1, 2, 3	any	No interface area reduction, i.e., $a_{fm} = 1$
negative	1	$a_{fm} = RP(6, NMAT)$
-1, -2, -3	0	$a_{fm} = S_\beta$
	2	$a_{fm} = S_\beta \cdot RP(7, NMAT)$
-4, -5, -6	0	$a_{fm} = k_{r\beta}$
	2	$a_{fm} = k_{r\beta} \cdot RP(7, NMAT)$
-10, -11, -12	0	$a_{fm} = S_e^{1+\gamma}$ (see Section 2.3)

a_{fm}	:	Fracture-matrix interface area reduction factor.
S_β	:	For flow of phase β, upstream saturation of phase β.
$k_{r\beta}$	:	For flow of phase β, upstream relative permeability of phase β.
$RP(6, NMAT)^\#$	:	6th parameter of rel. perm. function of upstream element.
$RP(7, NMAT)^\#$	:	7th parameter of rel. perm. function of upstream element.
#	:	If zero (i.e., not specified), reset to one.

Figure 2.1.1 shows the pseudo-code implemented for the interface area reduction calculation, revealing the control logic.

```
afm:=1
if ISO negative then
   determine material number NMAT of upstream gridblock
   if ISO=-1, -2, or -3 then
      afm:=upstream saturation
   else if ISO=-4, -5, or -6 then
      afm:=upstream relative permeability
   else if ISO=-10, -11, or -12 then
      afm:=Equation (2.3.6)
   end if
   if MOP(8)=1 then
      afm:=RP(6,NMAT)
   else if MOP(8)=2 then
      afm=afm*RP(7,NMAT)
   end if
end if
area:=area*afm
```

Figure 2.1.1. Pseudo-code for interface area reduction.

To validate whether the interface area available for fluid flow between two adjacent gridblocks is reduced from its geometric value by the corresponding factor described in Table 2.1.1, a one-dimensional, dual-permeability fracture-matrix model was developed with constant infiltration at the top and constant pressure and saturation at the bottom. The generic TOUGH2 input file is shown in Figure 2.1.2. The model has two layers, each layer with its own set of fracture and matrix properties. Note that the first four entries in block CONNE represent the connections between the fracture and matrix gridblocks, which will be subjected to interface area reduction. The different options are implemented by changing MOP(8), ISO, and AREA as described in the following sections.

Because of successful regression testing (see Section 2.9), the Run B simulations described below can be performed using either standard TOUGH2 or ITOUGH2 in forward mode.

```
Fracture-Matrix Interface Area Reduction
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
FRAC1    2    2000.0      0.10   1.0E-12   1.0E-12   1.0E-12       2.0     900.0

    7         0.5000    0.0100    1.0000                               0.01       0.1
    7         0.5000    0.0100 1.000E-04                1.000
MATR1    2    2000.0      0.10   1.0E-17   1.0E-17   1.0E-17       2.0     900.0
                        1.7300    0.2500
    7         0.2500    0.1000    1.0000                               0.01       0.1
    7         0.2500    0.1000 1.000E-05                1.000
FRAC2    2    2000.0      0.10   1.0E-12   1.0E-12   1.0E-12       2.0     900.0
                        1.7300    0.2500
    7         0.5000    0.0100    1.0000                               0.01       0.1
    7         0.5000    0.0100 1.000E-03                1.000
MATR2    2    2000.0      0.10   1.0E-16   1.0E-16   1.0E-16       2.0     900.0
                        1.7300    0.2500                               0.01       0.1
    7         0.2000    0.1500    1.0000
    7         0.2000    0.1500 1.000E-06                1.000

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM           123456789012345678901234
  -39999    99990000001100000000400003000
 1.000E-05            1.0E+06                            9.81

                0.8

ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1              10.1000E-010.1000E-01                              -.5000E+00
M   1              20.1000E+010.1000E+01                              -.5000E+00
F   2              10.1000E-010.0000E+00                              -.1500E+01
M   2              20.1000E+010.0000E+00                              -.1500E+01
F   3              30.1000E-010.0000E+00                              -.2500E+01
M   3              40.1000E+010.0000E+00                              -.2500E+01
F   4              30.1000E-010.0000E+00                              -.3500E+01
M   4              40.1000E+010.0000E+00                              -.3500E+01
F   5              3-.1000E-010.1000E-01                              -.4500E+01
M   5              4-.1000E+010.1000E+01                              -.4500E+01

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1M   1                    -10.0000E+000.5000E+000.1000E+01
F   2M   2                    -10.0000E+000.5000E+000.1000E+01
F   3M   3                    -10.0000E+000.5000E+000.1000E+01
F   4M   4                    -10.0000E+000.5000E+000.1000E+01
M   1M   2                     30.5000E+000.5000E+000.1000E+010.1000E+01
M   2M   3                     30.5000E+000.5000E+000.1000E+010.1000E+01
M   3M   4                     30.5000E+000.5000E+000.1000E+010.1000E+01
M   4M   5                     30.5000E+000.5000E+000.1000E+010.1000E+01
F   1F   2                     30.5000E+000.5000E+000.1000E-010.1000E+01
F   2F   3                     30.5000E+000.5000E+000.1000E-010.1000E+01
F   3F   4                     30.5000E+000.5000E+000.1000E-010.1000E+01
F   4F   5                     30.5000E+000.5000E+000.1000E-010.1000E+01

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1                                COM1 1.0000E-07

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
M   5
 0.99
F   5
 0.02

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 2.1.2. Generic TOUGH2 input file for validating fracture-matrix interface area reduction.

2.1.1 Interface Area Reduced by a Constant

To confirm that the interface area available for fluid flow between two adjacent gridblocks is reduced from its geometric value by the constant provided through TOUGH2 input variable RP(6,NMAT), the following two runs were performed:

Run A: Steady-state simulation with geometric interface area, using negative values for ISOT, setting MOP(8)=1, and setting RP(6,NMAT)=0.01 for all rock types. The input file is named *vvFM1A*; it is shown in Figure 2.1.2.

Run B: Steady-state simulation with interface areas reduced to 1% of their geometric values and positive ISOT. The input file is named *vvFM1B*; the CONNE block is reproduced in Figure 2.1.1.1.

Because of limited accuracy in specifying interface areas in the TOUGH2 input file, there may be slight differences in the two results. However, for the values chosen here, both runs should yield identical results.

The following command lines were used to run the test cases:

```
itough2 -v3.2 vvFM1A 9 &
itough2 -v3.2 vvFM1B 9 &
```

Inspection of the two output files *vvFM1A.out* and *vvFM1B.out* confirms that identical results were obtained, fulfilling Requirement 1.1.

```
CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F    1M    1                    10.0000E+000.5000E+000.1000E-01
F    2M    2                    10.0000E+000.5000E+000.1000E-01
F    3M    3                    10.0000E+000.5000E+000.1000E-01
F    4M    4                    10.0000E+000.5000E+000.1000E-01
M    1M    2                     30.5000E+000.5000E+000.1000E+010.1000E+01
M    2M    3                     30.5000E+000.5000E+000.1000E+010.1000E+01
M    3M    4                     30.5000E+000.5000E+000.1000E+010.1000E+01
M    4M    5                     30.5000E+000.5000E+000.1000E+010.1000E+01
F    1F    2                     30.5000E+000.5000E+000.1000E-010.1000E+01
F    2F    3                     30.5000E+000.5000E+000.1000E-010.1000E+01
F    3F    4                     30.5000E+000.5000E+000.1000E-010.1000E+01
F    4F    5                     30.5000E+000.5000E+000.1000E-010.1000E+01
```

Figure 2.1.1.1. Block CONNE of file *vvFM1B*, showing positive values for variable ISOT and interface areas reduced to 1% of the values shown in Figure 2.1.2.

2.1.2 Interface Area Reduced by Upstream Saturation

To confirm that the interface area available for fluid flow between two adjacent gridblocks is reduced from its geometric value by the saturation of the upstream gridblock, the following two runs were performed:

Run A: Steady-state simulation with geometric interface area, setting ISOT=-1, and MOP(8)=0. The input file is named *vvFM2A*; it is identical to the file shown in Figure 2.1.2, with the exception of MOP(8).

Run B: Steady-state simulation with interface areas specified directly in block CONNE, reduced by the steady-state upstream saturation calculated in Run A. The input file is named *vvFM2B*.

The results of the two runs are expected to be slightly different because (1) there is limited accuracy in specifying interface areas in the TOUGH2 input file, and (2) while the interface area available for flow changes with saturation (and thus with time) in Run A, the reduced value is fixed throughout Run B. This difference leads to a different system development as it evolves from its initial state towards steady-state conditions, with different time steps taken, different total simulation times to reach steady state, and different number of iterations, leading to different round-off and time-discretization errors. Nevertheless, the results at steady-state are expected to be very similar, with the maximum difference in any output variable being less than 0.1%.

The following command line was used for Run A:

```
itough2 -v3.2 vvFM2A 9 &
```

The saturations as written to the SAVE file *vvFM2A.sav* (see Figure 2.1.2.1) are used as reduction factors of the interface areas of the first four connections specified in the CONNE block of file *vvFM2B* as shown in Figure 2.1.2.2. At steady state, flow is from the fractures into the matrix, making the fracture gridblocks the upstream gridblocks.

```
INCON -- INITIAL CONDITIONS FOR    10 ELEMENTS AT TIME  0.429497E+16
F   1             0.10000000E+00
 0.4338920874502E+00 0.0000000000000E+00
M   1             0.10000000E+00
 0.8921064332228E+00 0.0000000000000E+00
F   2             0.10000000E+00
 0.6098054293383E+00 0.0000000000000E+00
M   2             0.10000000E+00
 0.8960659745952E+00 0.0000000000000E+00
F   3             0.10000000E+00
 0.2750228155389E+00 0.0000000000000E+00
M   3             0.10000000E+00
 0.9881525567958E+00 0.0000000000000E+00
F   4             0.10000000E+00
 0.1754130794552E+00 0.0000000000000E+00
M   4             0.10000000E+00
 0.9890779950707E+00 0.0000000000000E+00
F   5             0.10000000E+00
 0.2000000000000E-01 0.0000000000000E+00
M   5             0.10000000E+00
 0.9900000000000E+00 0.0000000000000E+00
+++
   34   89    4 0.10000000E-04 0.42949673E+16
```

Figure 2.1.2.1. File *vvFM2A.sav*, showing steady-state saturations obtained in Run A.

```
CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1M   1                    10.0000E+000.5000E+000.43389087
F   2M   2                    10.0000E+000.5000E+000.60980543
F   3M   3                    10.0000E+000.5000E+000.27502282
F   4M   4                    10.0000E+000.5000E+000.17541308
M   1M   2                    30.5000E+000.5000E+000.1000E+010.1000E+01
M   2M   3                    30.5000E+000.5000E+000.1000E+010.1000E+01
M   3M   4                    30.5000E+000.5000E+000.1000E+010.1000E+01
M   4M   5                    30.5000E+000.5000E+000.1000E+010.1000E+01
F   1F   2                    30.5000E+000.5000E+000.1000E-010.1000E+01
F   2F   3                    30.5000E+000.5000E+000.1000E-010.1000E+01
F   3F   4                    30.5000E+000.5000E+000.1000E-010.1000E+01
F   4F   5                    30.5000E+000.5000E+000.1000E-010.1000E+01
```

Figure 2.1.2.2. Block CONNE of file *vvFM2B*, showing interface areas reduced by the fracture saturations shown in Figure 2.1.2.1.

The following command line was used for Run B:

```
itough2 -v3.2 vvFM2B 9 &
```

Inspection of the two output files *vvFM2A.out* and *vvFM2B.out* confirms that identical results were obtained, fulfilling Requirement 1.2.

2.1.3 Interface Area Reduced by Upstream Saturation Times a Constant

To confirm that the interface area available for fluid flow between two adjacent gridblocks is reduced from its geometric value by the saturation of the upstream gridblock times the factor provided through variable RP(7,NMAT), the following two runs were performed:

Run A: Steady-state simulation with geometric interface area, setting ISOT=-1, and MOP(8)=2, and RP(7,NMAT)=0.1 for all rock types. The input file is named *vvFM3A*; it is identical to the file shown in Figure 2.1.2, with the exception of MOP(8).

Run B: Steady-state simulation with interface areas specified directly in block CONNE, reduced by the steady-state upstream saturation calculated in Run A times 0.1. The input file is named *vvFM3B*.

The results at steady-state are expected to be very similar, with the maximum difference in any output variable being less than 0.1%.

The following command line was used for Run A:

```
itough2 -v3.2 vvFM3A 9 &
```

The saturations as written to the SAVE file *vvFM3A.sav* (see Figure 2.1.3.1) are used as reduction factors of the interface areas specified for the first four connections in the CONNE block of file *vvFM3B* as shown in Figure 2.1.3.2. The interface areas are further reduced by 0.1, which is the factor specified in RP(7,NMAT) of Run A. At steady state, flow is from the fractures into the matrix, making the fracture gridblocks the upstream gridblocks.

```
INCON -- INITIAL CONDITIONS FOR    10 ELEMENTS AT TIME   0.429497E+16
F   1             0.10000000E+00
 0.4376531245338E+00 0.0000000000000E+00
M   1             0.10000000E+00
 0.8357579578799E+00 0.0000000000000E+00
F   2             0.10000000E+00
 0.6175860651419E+00 0.0000000000000E+00
M   2             0.10000000E+00
 0.8436032656234E+00 0.0000000000000E+00
F   3             0.10000000E+00
 0.2911632608216E+00 0.0000000000000E+00
M   3             0.10000000E+00
 0.9878238253713E+00 0.0000000000000E+00
F   4             0.10000000E+00
 0.1852263062714E+00 0.0000000000000E+00
M   4             0.10000000E+00
 0.9889180282040E+00 0.0000000000000E+00
F   5             0.10000000E+00
 0.2000000000000E-01 0.0000000000000E+00
M   5             0.10000000E+00
 0.9900000000000E+00 0.0000000000000E+00
+++
   35   89    4 0.10000000E-04 0.42949673E+16
```

Figure 2.1.3.1. File *vvFM3A.sav*, showing steady-state saturations obtained in Run A.

```
CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1M   1                    10.0000E+000.5000E+000.04376531
F   2M   2                    10.0000E+000.5000E+000.06175871
F   3M   3                    10.0000E+000.5000E+000.02911633
F   4M   4                    10.0000E+000.5000E+000.01852263
M   1M   2                    30.5000E+000.5000E+000.1000E+010.1000E+01
M   2M   3                    30.5000E+000.5000E+000.1000E+010.1000E+01
M   3M   4                    30.5000E+000.5000E+000.1000E+010.1000E+01
M   4M   5                    30.5000E+000.5000E+000.1000E+010.1000E+01
F   1F   2                    30.5000E+000.5000E+000.1000E-010.1000E+01
F   2F   3                    30.5000E+000.5000E+000.1000E-010.1000E+01
F   3F   4                    30.5000E+000.5000E+000.1000E-010.1000E+01
F   4F   5                    30.5000E+000.5000E+000.1000E-010.1000E+01
```

Figure 2.1.3.2. Block CONNE of file *vvFM3B*, showing interface areas reduced by 10% of the fracture saturations shown in Figure 2.1.3.1.

The following command line was used for Run B:

```
itough2 -v3.2 vvFM3B 9 &
```

Inspection of the two output files *vvFM3A.out* and *vvFM3B.out* confirms that identical results were obtained, fulfilling Requirement 1.3.

2.1.4 Interface Area Reduced by Upstream Relative Permeability

To confirm that the interface area available for fluid flow between two adjacent gridblocks is reduced from its geometric value by the relative permeability of the upstream gridblock, the following two runs were performed:

Run A: Steady-state simulation with geometric interface area, setting ISOT=-4, and MOP(8)=0. The input file is named *vvFM4A*; it is identical to the file shown in Figure 2.1.2, with the exception of MOP(8) and ISOT for the first four connections.

Run B: Steady-state simulation with interface areas specified directly in block CONNE, reduced by the steady-state upstream relative permeability calculated in Run A. The input file is named *vvFM4B*.

The results at steady-state are expected to be very similar, with the maximum difference in any output variable being less than 0.1%.

The following command line was used for Run A:

```
itough2 -v3.2 vvFM4A 9 &
```

The liquid relative permeabilities as written to the TOUGH2 output file *vvFM4A.out* (see Figure 2.1.4.1) are used as reduction factors of the interface areas of the first four connections specified in the CONNE block of file *vvFM4B* as shown in Figure 2.1.4.2. At steady state, flow is from the fractures into the matrix, making the fracture gridblocks the upstream gridblocks.

```
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
Case 4: Fracture-Matrix Interface Area Reduction: upstream rel. perm.

                              KCYC =   36  -  ITER =    1  -  TIME = 0.42950E+16

 ELEM.  INDEX   X1          DX1         K(LIQ.)
 F   1      1 0.43804E+00 0.00000E+00 0.63542E-02
 M   1      2 0.82310E+00 0.00000E+00 0.14249E-01
 F   2      3 0.61830E+00 0.00000E+00 0.34911E-01
 M   2      4 0.83338E+00 0.00000E+00 0.16522E-01
 F   3      5 0.29271E+00 0.00000E+00 0.92665E-03
 M   3      6 0.98779E+00 0.00000E+00 0.16919E+00
 F   4      7 0.18617E+00 0.00000E+00 0.10746E-03
 M   4      8 0.98890E+00 0.00000E+00 0.17829E+00
 F   5      9 0.20000E-01 0.00000E+00 0.26158E-09
 M   5     10 0.99000E+00 0.00000E+00 0.18831E+00

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

Figure 2.1.4.1. Excerpt from file *vvFM4A.out*, showing steady-state liquid relative permeabilities obtained in Run A.

```
CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1M   1                      10.0000E+000.5000E+000.63542E-2
F   2M   2                      10.0000E+000.5000E+000.34911E-1
F   3M   3                      10.0000E+000.5000E+000.92665E-3
F   4M   4                      10.0000E+000.5000E+000.10746E-3
M   1M   2                      30.5000E+000.5000E+000.1000E+010.1000E+01
M   2M   3                      30.5000E+000.5000E+000.1000E+010.1000E+01
M   3M   4                      30.5000E+000.5000E+000.1000E+010.1000E+01
M   4M   5                      30.5000E+000.5000E+000.1000E+010.1000E+01
F   1F   2                      30.5000E+000.5000E+000.1000E-010.1000E+01
F   2F   3                      30.5000E+000.5000E+000.1000E-010.1000E+01
F   3F   4                      30.5000E+000.5000E+000.1000E-010.1000E+01
F   4F   5                      30.5000E+000.5000E+000.1000E-010.1000E+01
```

Figure 2.1.4.2. Block CONNE of file *vvFM4B*, showing interface areas reduced by the fracture relative permeabilities shown in Figure 2.1.4.1.

The following command line was used for Run B:

```
itough2 -v3.2 vvFM4B 9 &
```

Inspection of the two output files *vvFM4A.out* and *vvFM4B.out* confirms that identical results were obtained, fulfilling Requirement 1.4.

2.1.5 Interface Area Reduced by Upstream Relative Permeability Times a Constant

To confirm that the interface area available for fluid flow between two adjacent gridblocks is reduced from its geometric value by the relative permeability of the upstream gridblock times the factor provided through variable RP(7,NMAT), the following two runs were performed:

Run A: Steady-state simulation with geometric interface area, setting ISOT=-4, MOP(8)=2, and RP(7,NMAT)=0.1 for all rock types. The input file is named *vvFM5A*; it is identical to the file shown in Figure 2.1.2, with the exception of MOP(8) and ISOT for the first four connections.

Run B: Steady-state simulation with interface areas specified directly in block CONNE, reduced by 10% of the steady-state upstream liquid saturation calculated in Run A. The input file is named *vvFM5B*.

The results at steady-state are expected to be very similar, with the maximum difference in any output variable being less than 0.1%.

The following command line was used for Run A:

```
itough2 -v3.2 vvFM5A 9 &
```

The liquid relative permeabilities as written to the TOUGH2 output file *vvFM5A.out* (see Figure 2.1.5.1) are used as reduction factors of the interface area specified in the CONNE block of file *vvFM5B* as shown in Figure 2.1.5.2. The interface areas are further reduced by 0.1, the factor specified in variable RP(7,NMAT) in Run A. At steady state, flow is from the fractures into the matrix, making the fracture gridblocks the upstream gridblocks.

```
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

Case 5: Fracture-Matrix Interface Area Reduction: upstream rel. perm.*factor

                                    KCYC =   35  -  ITER =    1  -  TIME = 0.53687E+16

 ELEM.  INDEX   X1           DX1         K(LIQ.)
 F    1      1 0.43834E+00 0.00000E+00 0.63752E-02
 M    1      2 0.80758E+00 0.00000E+00 0.11399E-01
 F    2      3 0.61896E+00 0.00000E+00 0.35104E-01
 M    2      4 0.81769E+00 0.00000E+00 0.13182E-01
 F    3      5 0.29408E+00 0.00000E+00 0.94738E-03
 M    3      6 0.98776E+00 0.00000E+00 0.16894E+00
 F    4      7 0.18700E+00 0.00000E+00 0.10976E-03
 M    4      8 0.98889E+00 0.00000E+00 0.17815E+00
 F    5      9 0.20000E-01 0.00000E+00 0.26158E-09
 M    5     10 0.99000E+00 0.00000E+00 0.18831E+00

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

Figure 2.1.5.1. Excerpt from file *vvFM5A.out*, showing steady-state liquid relative permeabilities obtained in Run A.

```
CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1M   1                    10.0000E+000.5000E+000.63752E-3
F   2M   2                    10.0000E+000.5000E+000.35104E-2
F   3M   3                    10.0000E+000.5000E+000.94738E-4
F   4M   4                    10.0000E+000.5000E+000.10976E-4
M   1M   2                     30.5000E+000.5000E+000.1000E+010.1000E+01
M   2M   3                     30.5000E+000.5000E+000.1000E+010.1000E+01
M   3M   4                     30.5000E+000.5000E+000.1000E+010.1000E+01
M   4M   5                     30.5000E+000.5000E+000.1000E+010.1000E+01
F   1F   2                     30.5000E+000.5000E+000.1000E-010.1000E+01
F   2F   3                     30.5000E+000.5000E+000.1000E-010.1000E+01
F   3F   4                     30.5000E+000.5000E+000.1000E-010.1000E+01
F   4F   5                     30.5000E+000.5000E+000.1000E-010.1000E+01
```

Figure 2.1.5.2. Block CONNE of file *vvFM5B*, showing interface areas reduced by 10% of the fracture liquid relative permeabilities shown in Figure 2.1.5.1.

The following command line was used for Run B:

```
itough2 -v3.2 vvFM5B 9 &
```

Inspection of the two output files *vvFM5A.out* and *vvFM5B.out* confirms that identical results were obtained, fulfilling Requirement 1.5.

2.2 Free Drainage Boundary Condition

A free drainage boundary condition for liquid flow is implemented, in which gravity is the only driving force, i.e., (capillary) pressure gradients are ignored across the interface to a boundary gridblock. This type of boundary condition comes into effect at each connection, in which one of the gridblocks belongs to rock type DRAIN.

To test whether the free drainage boundary condition is correctly implemented, one-dimensional, gravity-driven, unsaturated flow is calculated with a free drainage boundary condition at the bottom of the column. If the resulting steady-state saturation profile is uniform and not affected by the capillary pressure gradient to the boundary gridblock, the implementation is considered correct.

The TOUGH2 input file is shown in Figure 2.2.1. Note that the last element is inactive (negative volume) and associated with rock type DRAIN.

The following command line was used for Run B:

```
itough2 -v3.2 vvFDBC 9 &
```

The steady-state solution (TOUGH2 output file *vvFDBC.out*) is shown in Figure 2.2.2. Note that the boundary gridblock would act as a capillary barrier, leading to a saturation buildup and thus nonuniform saturation profile. However, as a result of the newly implemented free drainage boundary condition, the saturation profile is uniform, fulfilling Requirement 2.

```
Free drainage boundary condition
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
FRACT    2    2000.0       0.10   1.0E-12   1.0E-12   1.0E-12       2.0     900.0

    7         0.5000    0.0100    1.0000                           0.01       0.1
    7         0.5000    0.0100 1.000E-04                1.000
DRAIN    2    2000.0       0.10   1.0E-12   1.0E-12   1.0E-12       2.0     900.0

    7         0.5000    0.0100    1.0000                           0.01       0.1
    7         0.5000    0.0100 1.000E-04                1.000

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM          1234567890123456789012345678901234
   -39999   9999000000110000000400003000
 1.000E-05           1.0E+06                             9.81

                0.5
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1    1    1    6

ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1              10.1000E+000.1000E-01                                -.5000E+01
F   2              10.1000E+000.0000E+00                                -.1500E+02
F   3              10.1000E+000.0000E+00                                -.2500E+02
F   4              10.1000E+000.0000E+00                                -.3500E+02
F   5              2-.1000E+000.1000E-01                                -.4500E+02

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1F   2                    30.5000E+010.5000E+010.1000E-010.1000E+01
F   2F   3                    30.5000E+010.5000E+010.1000E-010.1000E+01
F   3F   4                    30.5000E+010.5000E+010.1000E-010.1000E+01
F   4F   5                    30.5000E+010.5000E+010.1000E-010.1000E+01

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1                              COM1 1.0000E-07

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 2.2.1. TOUGH2 input file *vvFDBC* for free drainage boundary problem.